COMPARATIVE STUDY OF NUMERICAL SCHEMES USED FOR ONE-DIMENSIONAL TRANSPORT MODELLING

Attila Gajdos[1]
Technical University of Budapest, Department of Water Resources Engineering
H-1111 Budapest
Stéphane Mandelkern[2]
National Hydraulic Laboratory - Electricité de France, River Hydraulic Group
F-78401 Chatou

SUMMARY

The focus is on the advection term in this paper. The scope is to give a comparative evaluation of numerical schemes. The investigated methods are submitted to different tests with several initial distributions and hydraulic conditions. The emphasis is on high order accurate methods, like the finit volume based QUICKEST and the caracteristics based Holly-Preissmann and HYP1FA schemes.

Keywords: solute transport, advection-dispersion equation, numerical schemes

1. INTRODUCTION

The equation of mass transport is used to simulate such environmental problems, like contaminant spreading in rivers. In most of the cases the 3D phenomenon can be simplified to 1D problem. This supposes that the contaminant has already been well mixed in both transversal and vertical directions. This approach is really considered as third phase of matter mixing, where the phases, provided a point source of pollution are the following (van Mazijk, 1996, Jobson, 1997): in the first phase vertical mixing (completed within 50-100 average river depths) is predominant. In the second phase transversal mixing over the cross sectional area of the river (completed within 100-300 river widths) is predominant. The transversal mixing distance is sometimes very long, therefore the second phase is often not separated from the third phase, in which the longitudinal mixing is predominant.

The 1D transport equation in conservative formulation (Mandelkern, van Haren, 1995):

$$\frac{\partial (cA)}{\partial t} + \frac{\partial (ucA)}{\partial x} = \frac{\partial}{\partial x}\left(A \cdot K \frac{\partial c}{\partial x} \right) + (q_s - q_b)\frac{A}{h} + S_c \cdot A \qquad (1.1)$$

[1] PhD student
[2] Research Engineer

where $c(x,t)$: concentration, (g/m^3)
$A(x,t)$: wet section, (m^2)
$u(x,t)$: velocity of the stream, (m/s)
$K(x,t)$: dispersion coefficient, (m^2/s)
$h(x,t)$: water depth, (m)
$q_s(x,t), q_b(x,t)$: surface source on the surface and the bottom, $(g/m^2 s)$
$S_c(x,t)$: point source, $(g/m^3 s)$

Substituting the continuity equation (1.2) of the stream into the above equation,

$$\frac{\partial A}{\partial t} + \frac{\partial u A}{\partial x} = 0 \tag{1.2}$$

equation 1.1 can be rewritten in the non-conservative form:

$$\frac{\partial c}{\partial t} + u \frac{\partial c}{\partial x} = \frac{1}{A} \frac{\partial}{\partial x} \left(A \cdot K \frac{\partial c}{\partial x} \right) + \frac{(q_s - q_b)}{h} + S_c \tag{1.3}$$

Although the one-dimensional advection-dispersion equation seems simple, accurate modelling of mass transport often meets difficulties. Analytical solution exists for a limited number of problems only, with restrictions for initial condition and coefficients (Zoppou, Knight, 1997). To avoid these restrictions numerical methods are used to solve the above equation. Generally, numerical solution of the advection-dispersion equation happens in two stages within one timestep. This widely used method is called "split operator approach" (Komatsu, Ohgushi, Asai, 1997). In the first stage pure advection is taken into account and in the second stage pure dispersion process is solved. One of the most serious problems is accurate modelling of the advection term. Problems of artificial dispersion or viscosity, difficulties in the surroundings of sudden gradient changes, phase errors etc. Proper modelling of the 2nd stage or dispersion term needs less effort.

In case of pure advection without source term, equation 1.1 and equation 1.3 become:

$$\frac{\partial (cA)}{\partial t} + \frac{\partial (ucA)}{\partial x} = 0 \qquad \text{(conservative form)} \tag{1.4}$$

$$\frac{\partial c}{\partial t} + u \frac{\partial c}{\partial x} = 0 \qquad \text{(non-conservative form)} \tag{1.5}$$

In this study 6 explicit and 3 implicit schemes, based on different theoretical background are investigated to present a comparative study by solving the advection equation. Applied explicit schemes: first order upwind, second order upwind, Lax-Wendroff, Fromm’s method, QUICKEST (Leonard, 1997), Holly-Preissmann (Holly, Preissmann, 1977). Implicit schemes: Crank-Nicolson (Wang, Lacroix, 1997), Implicit QUICK (Chen, Falconer, 1992), HYP1FA (Hervouet, 1986).

2. TEST CASES WITH ANALYTICAL SOLUTIONS

Supposing a unit width and depth channel where the velocity is constant along the length, the conservative and non-conservative advection equations (1.4, 1.5) can be written in the same form, which is equivalent to equation 1.5.

$$\frac{\partial c}{\partial t} + u\frac{\partial c}{\partial x} = 0 \tag{2.1}$$

The exact solution of the above equation for a given initial condition is the following:

$$c(x,t) = c(x - u \cdot t, 0) \tag{2.2}$$

where the initial condition is c(x,0).

To get view about the behaviours of the schemes, equation 2.1 was solved numerically for different initial conditions with both smoothly changing concentration gradient and abrupt gradient changes (Islam, Chaudhry, 1997, Leonard, 1991).

Uniform grid was chosen, dx=100 m in space and dt=50 s in time. Different velocities were applied, u=1.0 m/s and u=1.8 m/s, so the Courant number ($\alpha = u\Delta t/\Delta x$) was α=0.5 and α=0.9.

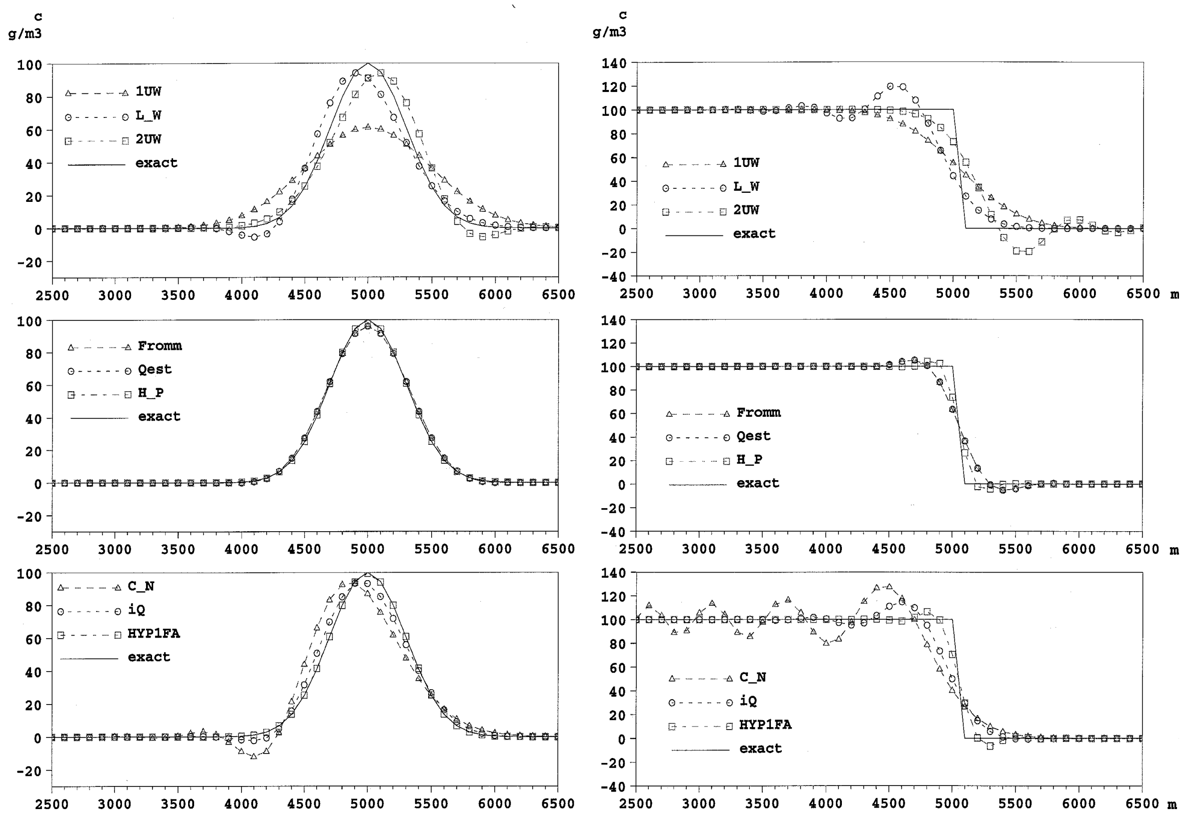
One of the initial conditions was a gaussian distribution, where the concentration is described by the following form:

$$C(x,t) = C_0 \exp\left[-\frac{(x - x_0 - ut)^2}{2\sigma^2}\right] \tag{2. 3}$$

C_0 - maximum concentration, (g/m^3)
x_0 - position of C_0 at time t_0, (m)
σ - standard deviation, (m).

To survey the behaviours of the schemes for increasing gradient changes, the standard deviation of the concentration distribution was decreased from σ = 500 m via σ = 300 m to σ = 100 m. This means that the 3σ region (practically the whole contaminant cloud) was covered by 31, 19 and 7 nodes according to the value of σ. The upstream and downstream boundary conditions were zero.

Other initial condition was a step profile, where C_0 was the concentration of the upper plateau, and the downstream concentration was zero. The upper boundary condition was C_0, while the lower boundary was zero.
Box or trapesoidal profiles are also used in the literature, but for highly oscillatory schemes the oscillations caused by step-up interfere with those of step-down, resulting complex wavepattern. The step profile is also basic test of monotonicity, a main aspect



The results indicate that every scheme is sensitive to the resolution of the concentration front (for example gaussian distribution with σ = 100 or σ = 500 m in the tests).

The first order upwind scheme is not able to describe faithfully any advection term, because of the strong artificial diffusion effect. This scheme has a unique ability, it is free from wiggles or under and over estimations. The Lax-Wendroff and second order upwind schemes have similar properties. They have significant phase errors, namely phase-lead (second order upwind) or phase-lag (Lax-Wendroff), oscillations in the vicinity of abrupt gradient changes. The advantage of second order upwind against Lax-Wendroff scheme is, that it is stable up to $\alpha = 2$, while the latter one is stable only if $\alpha \leq 1$. The phase-lead and phase-lag effect was eliminated by the construction of Fromm's method. It gives good solutions, which are just a little bit worse, than those of the 3rd order QUICKEST scheme. QUICKEST produces very good results in most of the tests, although for small σ gaussian distribution it does not give satisfactory solution, either.

The Holly-Preissmann scheme is one of the most accurate among the schemes involved in this study. It gives very good solutions even for sharp fronts. Its drawback against the also accurate scheme HYP1FA is, that the Holly-Preissmann method is limited to the Courant number. On the other hand HYP1FA sometimes produces small oscillations at the downstream side of sudden gradient changes.

It seems, that some inconditionally stable schemes which are not limited to the Courant number (according to the stability analysis) have real restriction in precise modelization of the examined phenomena. The Crank-Nicolson scheme gives poorer and poorer result for increasing Courant number. Besides it produces very long and large amplitude oscillations behind abrupt gradient changes. The implicit QUICK also gives worse and worse result with increase of the Courant number, similarly to the Crank-Nicolson scheme, although in smaller extent.

3. TEST CASE FOR THE RIVER VIENNE

In this test case a simple adaptation is introduced for the river Vienne. The computation domain was between Civaux and tributary Creuse. The river is canalized, with several barrages along the length. The average discharge at Civaux is 86 m^3/s, calculated from the period 1965-1989. In about 50 % of the summer days the discharge does not exceed 30 m^3/s.

In the test case steady state hydraulic condition was supposed, $Q = 40\ m^3/s$ as the upper boundary condition at Civaux, and z = 35 m.a.s.l. (NGF) as the lower boundary condition at tributary Creuse. The applied discharge corresponds to a dry period for the river. Internal conditions were considered at the barrages, based on the function of discharge and waterheight relation. The computation of steady hydraulic state was carried out by LIDO system, a 1D flow modelling software developped at the River Hydraulic Group of the National Hydraulic Laboratory of EDF. According to the computation, the velocity as well as the wet section is strongly varying along the river, the average velocity is less than 0.4 m/s.

In order to compute contaminant transport the following conditions were used for TRACER module (part of LIDO system, dedicated to transport and dispersion of passive tracers). At t_0 time of computation the initial condition was a gaussian type distribution with standard deviation of 300 m. Practically speaking, the pollution cloud was approximately 2000 m long. The maximum concentration was 1 g/m^3 at the section of 30 026 m. The boundary conditions were zero.
Three numerical schemes which proved to be the most accurate during the tests were applied to the computation, namely HYP1FA, the Holly-Preissmann and QUICKEST schemes. The timestep was 30 s in the cases, which is a small value in practical aspect.

In the first case pure advection, in the second case advection-dispersion process with a small and constant dispersion coefficient ($K = 5\ m^2/s$) were applied along the river. The results obtained in the test are shown in Fig. 2.

The pure advection resulted rather different contaminant distributions. Each scheme has some drawback. HYP1FA produces small disorders at the upstream foot of the distribution. The Holly-Preissmann scheme has just a little underestimation at the foot of the concentration front, but the computed contaminant mass along the domain changes in the biggest extent. QUICKEST shows about 25% degradation of the maximum concentration and slight underestimation at the foot.

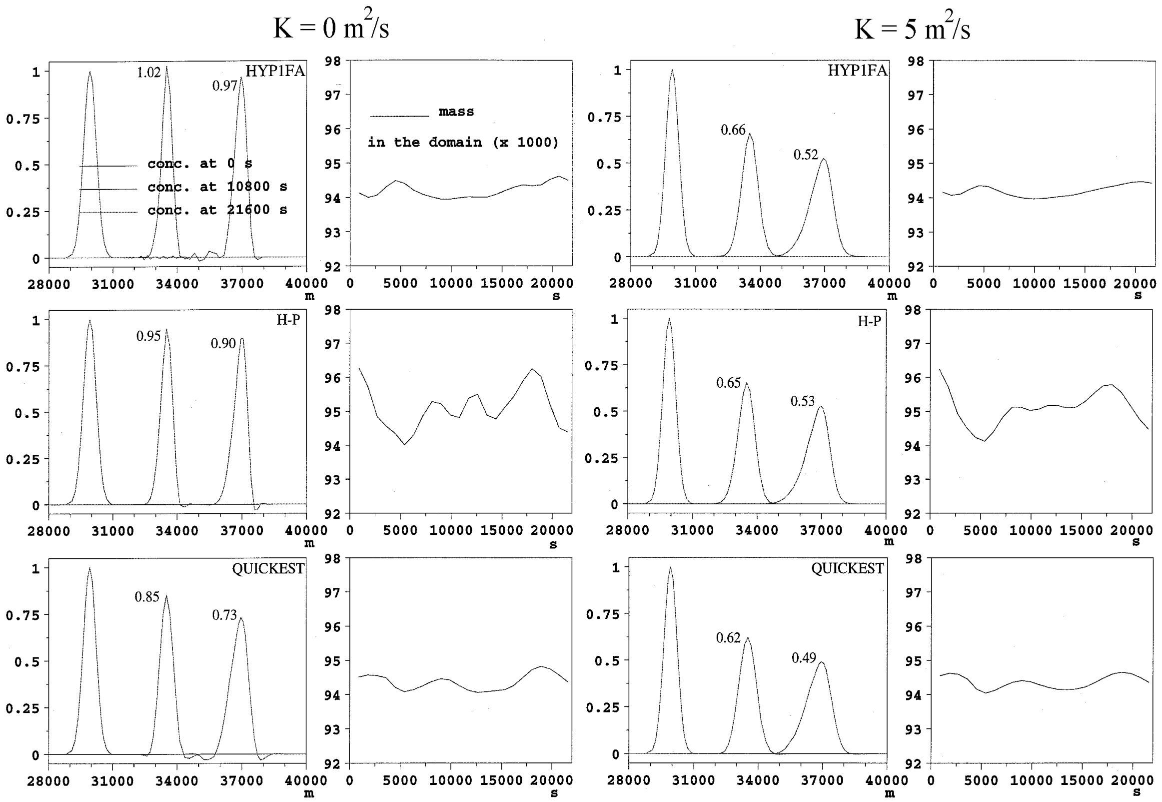


Fig. 2. Concentration and mass in the domain.

Regarding the advection-dispersion process, it is seen that the results became very similar. The dispersion term decreases the over and underestimations. At K=5 m^2/s, only QUICKEST produced very small underestimation at the foot of the contaminant cloud. The effect caused by dispersion depends on the Peclet number $P_\Delta = \dfrac{u\Delta x}{K}$ (Wang, Lacroix, 1997), that is the ratio of the advective and dispersive terms. If $P_\Delta \rightarrow \infty$ the advection, if $P_\Delta \rightarrow 0$, the dispersion term is dominant. Depending on the value of the dispersion, some of the schemes detailed in the previous chapter could also give satisfactory solutions.

The calculated mass in the domain as function of time did not change in character by the presence of dispersion, that is during the computation period the mass of contaminant calculated from the results given by the Holly Preissmann scheme varied in the biggest extent. It is also remarkable, that there was no sharp difference in amplitudes between the theoretically non conservative HYP1FA and the conservative QUICKEST schemes. During calculations TRACER uses velocity and wet section data computed by LIDO which satisfy the continuity on high level due to the applied numerical method. Therefore the application of the non-conservative HYP1FA and Holly-Preissmann schemes does not cause problem.

The computation time was also examined during the tests, comparing the three most accurate methods. As a rough estimation it was observed, that the Holly-Preissman scheme is about three times while QUICKEST is approximately twice faster than

HYP1FA. Although HYP1FA is more flexible in the sense of stability, being not limited to the Courant number.

4. CONCLUSIONS

The main part of this study was dedicated to advective transport. The investigated methods were submitted to different tests in order to compare their properties and accuracies in simple and real cases.

Considering the results of the five finit volume formulated explicit schemes, QUICKEST proves its superiority over the four other schemes. It is free from the disagreeable nonphysical oscillatory and phase error properties of the Lax-Wendroff and second order upwind schemes, although it also produces small under and overestimations in the vicinity of sudden gradient changes. Being based on quadratic upstream interpolation QUICKEST is more accurate - using the same nodes -, than the linear interpolation based Fromm's method which was developed to reduce the phase errors and oscillations of the Lax-Wendroff and second order upwind schemes. The under and over estimations of the before mentioned higher order flux based schemes can be eliminated by the ULTIMATE strategy (Leonard, 1991), for example. The first order upwind method is not suitable for any accurate application, it served as comparative base.

The finit volume based time centered implicit QUICK proved to be more precise than the traditional implicit Crank-Nicolson scheme. Although they are not limited to the Courant number, their accuracy strongly worsen with the increase of the Courant number. The schemes are highly oscillatory in case of pure advection.

The caracteristics based explicit Holly-Preissmann and implicit HYP1FA methods gave very good and similar results in general, the Holly-Preissmann scheme proved slightly better only for extreme initial distributions (for example step front). The HYP1FA, similarly to the above mentioned implicit methods is unconditionally stable, with a great advantage, namely it is free from the growing oscillation for higher Courant number appeared at the Crank-Nicolson and implicit QUICK schemes.

Finally, HYP1FA, the Holly-Preissmann and QUICKEST schemes were adapted to TRACER module, and simulations were carried out for the river Vienne. In the first case dispersion term was not taken into account. Each scheme showed some disadvantageous property. HYP1FA presented small disorders at the foot of the distribution, the Holly-Preissmann scheme was the most sensitive in the aspect of mass-conservation, while QUICKEST produced significant degradation with underestimations at the foot of the concentration. In the second case a relatively small dispersion term was applied. Due to its stabilizing effect the small over and underestimations disappeared or decreased, and the calculated concentration distributions became very similar. This means, that other investigated, but less accurate schemes can also present solutions close to a desired accuracy.

As a final consequence it looks, that there is no at all points better scheme among the three examined high order schemes. In a sense there is better method, which in other sense shows defect against the others. However, because the applied dispersion value in the testcase for the river Vienne can be considered as a lower limit of the dispersion in rivers, it seems that in practical cases all the three highly accurate schemes give satisfactory solutions.

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